

Propyl carbamate
627-12-3 | DTXSID7060833

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 68.3 °C

Global applicability domain: Inside

Local applicability domain index: 7.28e-01

Confidence level: 7.16e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Propyl carbamate</div> <div>Measured: 60.0</div> <div>Predicted: 68.3</div>	<div>Image not found</div> <div>Isopropyl carbamate</div> <div>Measured: 93.0</div> <div>Predicted: 74.3</div>	<div>Image not found</div> <div>Carbamic acid, butyl ester</div> <div>Measured: 53.0</div> <div>Predicted: 64.5</div>
<div>Image not found</div> <div>Carbamic acid, 2-methylpropyl ester</div> <div>Measured: 67.0</div> <div>Predicted: 66.9</div>	<div>Image not found</div> <div>Urethane</div> <div>Measured: 49.0</div> <div>Predicted: 55.3</div>	